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Metal-insulator transition in a disordered two-dimensional electron gas including temperature effects

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We calculate self-consistently, the mutual dependence of electron correlations and electron-defect scattering for a two-dimensional electron gas at finite temperature. We employ a Singwi, Tosi, Land, and Sjölander approach to calculate the electron correlations, while the electron scattering rate off Coulombic impurities and surface roughness is calculated using self-consistent current-relaxation theory. The methods are combined and self-consistently solved. We discuss a metal-insulator transition for a range of disorder levels and electron densities. Our results are in good agreement with recent experimental observations. [S0163-1829(99)00511-1]

In recent experiments[1,2] on two-dimensional electronic systems in zero-magnetic field, a well-defined metal-insulator transition has been observed. The transition contradicts the prediction[3] that two-dimensional electron systems are always localized in the presence of any disorder. The mobility is large at the transition point ($\mu > 1$ m^2/Vs). For such high mobilities the scattering off defects is weak and the correlations between electrons are significant.

Both disorder and correlations by themselves can lead to at least two different types of localization. In the presence of disorder, Abrahams *et al.*[3] showed that noninteracting electrons in two dimensions cannot sustain static conductivity no matter how small the level of disorder is. On the other hand, if there are strong correlations between the charge carriers this can cause a different type of localization in disorder-free systems, which is associated with Wigner crystallization.[4] In real systems there are both electron-electron and electron-impurity interactions. With weak disorder and in the low electron density limit, the electron-electron interactions should dominate leading to Wigner crystallization, while in the high electron density limit, the electron correlations are very weak and the localization should be of the Anderson type. Between these two extremes, disorder and correlations compete with each other to decide the nature of the localization.

In this paper, we examine the interdependence of correlations and defect scattering at finite temperatures. We use the self-consistent formalism of Singwi, Tosi, Land, and Sjölander[5] (STLS) to treat electron-electron correlations, while for the electron-defect scattering we use a memory function approach[6] to calculate the decay time of the density fluctuations from scatterings off defects. Previous calculations of the influence of disorder have either used the first-Born approximation or else they have introduced an adjustable parameter γ for the electron scattering rate from the disorder. In these approaches the scattering rate is not affected by correlations, while the two effects are in fact interdependent and should be self-consistently linked.

For interacting carriers the linear response function is given by the random-phase approximation (RPA). In this ap-

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proach, the Coulomb correlations between the carriers is completely neglected. Many-body interactions modify the strength of the static Coulomb potential $V(q)=2\pi e^2/q\epsilon$. In the STLS formalism, the many-body correlations are taken into account by introducing a static local field $G(q)$. In the RPA expression for the response function, the bare $V(q)=2\pi e^2/q\epsilon$ is replaced by $V(q)[1-G(q)]$, and the response function becomes

$$\chi(q,\omega)=\frac{\chi^{(0)}(q,\omega)}{1+V(q)[1-G(q)]\chi^{(0)}(q,\omega)},\tag{1}$$

where $\chi^{(0)}(q,\omega)$ is the two-dimensional dynamical susceptibility for noninteracting electrons. We assume only the lowest energy subband is occupied.

We consider scattering from disorder that consists of a random distribution of Coulombic impurities of density n_i and interface surface roughness. The effect of disorder is to damp the charge-density fluctuations and this modifies the response function. Damping changes $\chi^{(0)}(q,\omega)$ to $\chi^{(s)}(q,\omega)$ given by[7]

$$\chi^{(s)}(q,\omega)=\frac{\chi^{(0)}(q,\omega+i\gamma)}{1-\dfrac{i\gamma}{\omega+i\gamma}\left[1-\dfrac{\chi^{(0)}(q,\omega+i\gamma)}{\chi^{(0)}(q)}\right]}.\tag{2}$$

In Eq. (2), the strength of the damping is represented by the scattering rate γ. At zero temperature in the diffusive regime $\chi^{(s)}(q,\omega)$ reduces to the well-known diffusive form $\lim_{\omega,q\to 0}\chi^{(s)}(q,\omega)=(2m^\star)/(\pi k_F\hbar^2)(\mathcal{D}q^2)/(\mathcal{D}q^2+\mathrm{i}\omega)$, where $\mathcal{D}=v_F^2/\gamma$ is the diffusion constant. In the limit when γ goes to infinity the system becomes nondiffusive. This represents a localized phase.[8] Using the Drude expression, γ is related to the mobility $\mu=e/(m^\star\gamma)$, where $m^\star$ is the effective mass.

Within the memory-function formalism[9] developed for electron scattering from disorder[6] the scattering rate γ can be determined from the imaginary part of the force-force relaxation function in the limit $(q,\omega)\to 0$. γ is expressed in terms of the carrier-disorder potential and the relaxation spectrum $\phi_0(q,i\gamma)=(1/i\gamma)[\chi^{(0)}(q,i\gamma)-\chi^{(0)}(q)]$ for noninteracting carriers scattering off the disorder,

$$i\gamma=-\frac{1}{2m^\star n_c}\sum_q q^2\frac{1}{\epsilon(q)^2}[n_i\langle|U_{\mathrm{imp}}(q)|^2\rangle+\langle|W_{\mathrm{surf}}(q)|^2\rangle]\times\frac{\phi_0(q,i\gamma)}{1+i\gamma\phi_0(q,i\gamma)/\chi^{(0)}(q)},\tag{3}$$

where n_c is the carrier density. The carrier-disorder potential is written in terms of $U_{\mathrm{imp}}(q)$, which is the impurity potential and $W_{\mathrm{surf}}(q)$, which represents surface roughness scattering at the interface. The screening of the disorder potential is given by $\epsilon(q)=1+V(q)[1-G(q)]\chi^{(s)}(q)$. The $G(q)$ takes into account correlations in the disordered system.

We take $U_{\mathrm{imp}}(q)=[(2\pi e^2)/(\epsilon q)]\exp(-qd)F_i(q)$ for monovalent Coulomb impurities that are in a layer separated from the electron or hole plane by distance d. We use for the impurity form factor $F_i(q)$ Eq. (4.28) in Ref. 10. For elec-

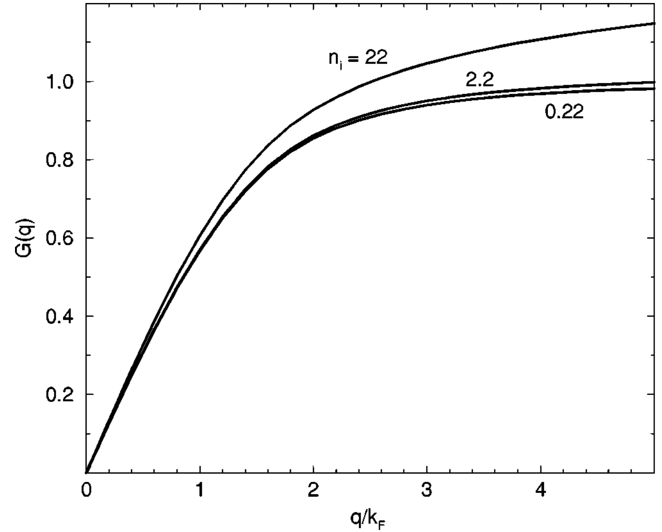

FIG. 1. Local-field factor $G(q)$ for different impurity densities (in units of 10^{11} cm^{-2}). The impurities are separated from the carrier plane by $d=5a_0^\star$. Carrier density is $n_c=35\times 10^{10}$ cm^{-2}.

trons in the Si metal-oxide semiconductor field-effect transistor (MOSFET's) we include interface surface roughness scattering $W_{\mathrm{surf}}(q)=\sqrt{\pi}\Delta\Lambda\Gamma(q)\exp(-(q\Lambda)^2/8)$. Values for the parameters $\Lambda=0.37$ nm and $\Delta=2.0$ nm are taken from Si MOSFET data.[11] For $\Gamma(q)$ we use the expression in Ref. 12. For GaAs surface roughness scattering is much smaller and we set $W_{\mathrm{surf}}(q)=0$.

In the STLS formalism, the density-density correlation function $\langle\delta\hat{n}(r,t)\delta\hat{n}(r',t)\rangle$ is approximated by the nonlinear product $\delta n(r,t)\times g(r-r')\times\delta n(r',t)$. The $\delta n(r,t)$ are expectation values and $g(r)$ is the pair-correlation function giving the probability of finding electrons a distance r apart. Using $g(r)=1+n_c^{-1}\int d^2\boldsymbol{q}\exp(i\boldsymbol{q}\cdot\boldsymbol{r})[S(q)-1]$, this gives us a relation between the static structure factor $S(q)$ and the local-field factor $G(q)$,

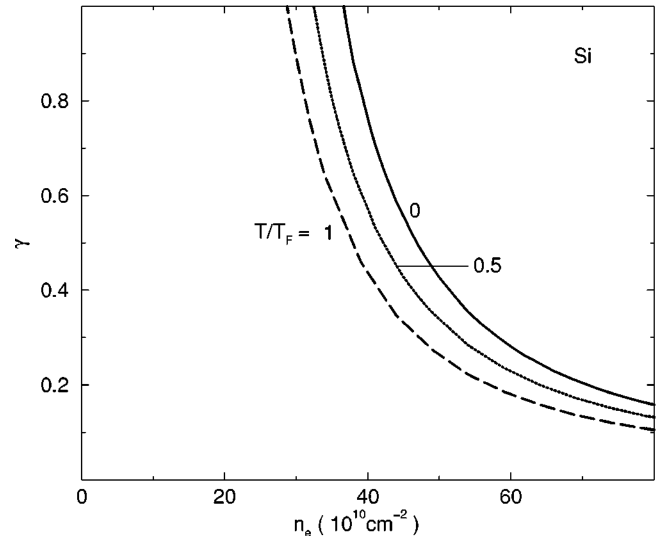

FIG. 2. Scattering rate γ for Si as a function of electron density n_e for impurity density 0.5×10^{11} cm^{-2}. Separation of the impurity layer is $d=a_0^\star$. Curves are for temperatures T (labels are in units of the Fermi temperature T_F for density n_e).

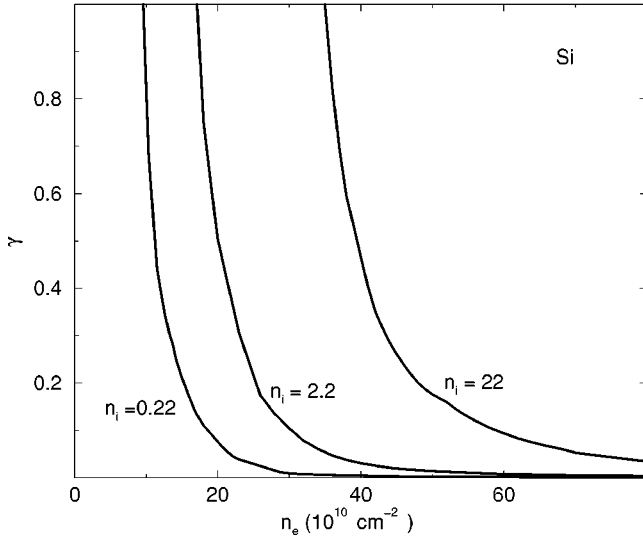

FIG. 3. Scattering rate γ for Si at $T=0$ as a function of electron density n_e. Curves are labeled for different impurity densities n_i (in units of 10^{11} cm^{-2}). Impurity separation $d=5a_0^\star$.

$$G(q)=-\frac{1}{n_c}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{(\boldsymbol{q}\cdot\mathbf{k})}{q^2}\frac{V(k)}{V(q)}[S(|\boldsymbol{q}-\boldsymbol{k}|)-1], \quad (4)$$

where $S(q)=(n_c\pi)^{-1}\int_0^\infty d\omega\,\mathrm{Im}\,\tilde{\chi}(q,\omega)$ is calculated from the fluctuation-dissipation theorem, and $\tilde{\chi}(q,\omega)$ is our total response function,

$$\tilde{\chi}(q,\omega)=\frac{\chi^{(s)}(q,\omega)}{1+V(q)[1-G(q)]\chi^{(s)}(q,\omega)}. \quad (5)$$

Starting from a given γ and $\chi^{(s)}(q,\omega)$ we use STLS to calculate the local field $G(q)$ in the presence of the disorder. We insert this in $\epsilon(q)$ to determine a new γ in Eq. (3), which defines a new $\chi^{(s)}(q,\omega)$ in Eq. (2), and the process recommences. This is repeated until there is overall self-consistency. The temperature dependence in our calculation enters through $\chi^{(s)}(q,\omega)$. The equations are solved at finite temperature for system parameters carrier density n_c, impurity density n_i, and remote impurity spacer layer separation d.

Through $\chi^{(s)}(q,\omega)$, Eqs. (4) and (5) build in the dependence of correlations on the defect scattering rate γ. Equation (3) gives the dependence of γ on the correlations through the $\epsilon(q)$. Thus taken together, these equations give us the mutual interdependence of correlations and the defect scattering rate.

Figure 1 shows the dependence of the local-field factor $G(q)$ on the impurity concentration at zero temperature. Increasing the disorder enhances $G(q)$. This is caused by the decrease in $\chi^{(s)}$ as the scattering rate γ gets bigger [Eq. (2)]. Enhancing $G(q)$ weakens the effective interaction between the carriers, and hence weakens the screening of the carrier-impurity potential. The net result of enhancing $G(q)$ is thus to strengthen the effect of the disorder potential. This in turn further increases γ. At a critical level of disorder this nonlinear feedback causes γ to increase rapidly and diverge. This leads to localization of the carriers.

TABLE I. Dependence on temperature of the critical carrier density for localization in Si. Impurity density $n_i=0.5\times10^{11}$ cm^{-2}. Impurities are embedded in the carrier plane.

T (K)	0	1	10	20
n_e (cm^{-2})	37×10^{10}	37×10^{10}	32×10^{10}	29×10^{10}

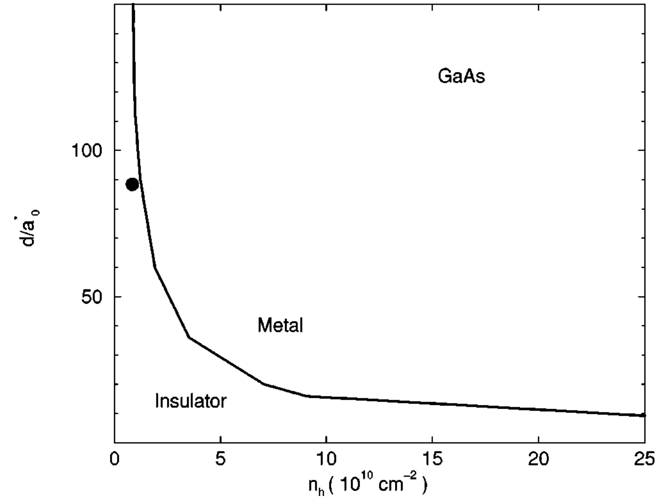

FIG. 4. Phase diagram for holes in GaAs. Critical hole density n_h at which $\gamma=1$ as a function of impurity layer separation d. Impurity density is $n_i=22\times10^{11}$ cm^{-2}. The experimental data point for GaAs is from Ref. 2.

We see this nonlinear behavior in Fig. 2. At a certain critical carrier density the scattering rate γ starts to increase rapidly. The impurity density here is $n_i=0.5\times10^{11}$ cm^{-2}, with the impurities separated from the carrier plane by distance $d=a_0^\star$ (the effective Bohr radius). The nonlinear increase in γ is due (i) to the enhancement of the local field $G(q)$, which strengthens the disorder potential, and (ii) to the rapid increase with γ of the total relaxation spectrum

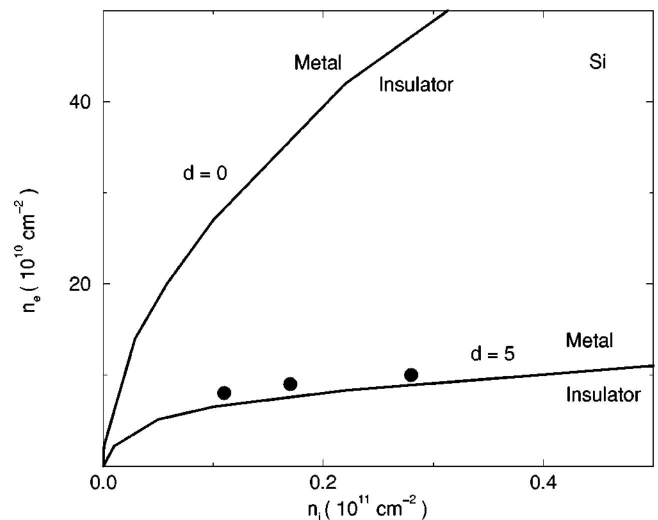

FIG. 5. Phase diagram for electrons in Si. Critical electron density n_e at which $\gamma=1$ as a function of impurity density for separations $d=0$ and $5a_0^\star$. The experimental data points are taken from Ref. 13.

$\phi_0(q,i\gamma)[1+i\gamma\phi_0(q,i\gamma)/\chi^{(0)}(q)]^{-1}$ [see Eq. (3)]. Figure 2 also shows the dependence of γ on temperature. The labels on the curves give the temperature in units of the Fermi temperature $T_F=E_F/k_B$ for density n_e. The metal-insulator transition is observed at carrier densities that are relatively low by conventional semiconductor standards so the Fermi temperature can be of the order of a few degrees K. We find γ diminishes with increasing temperature. This reflects the weakening of the correlations at finite T.

In Fig. 3 we show the increase of γ with impurity density at $T=0$. The curve labels give n_i in units of 10^{11} cm^{-2}. The impurity separation is $d=5a_0^\star$. As expected, increasing the impurity concentration has the effect of increasing the scattering rate. On the other hand, increasing the carrier density has the opposite effect on γ because the correlations are reduced. However, the nonlinear effects from n_e are much stronger than the nonlinear effects from n_i.

The metallic phase in the experimental systems is characterized by mean-free paths $lk_F \gg 1$, while in the localized phase $lk_F \lesssim 1$. We take the localization boundary to be the point where lk_F passes through unity. Table I gives for different temperatures the critical electron density at which $lk_F=1$. When the system is at finite temperature the correlations are reduced and one needs to go to slightly lower carrier densities before localization can be achieved.

Table I shows the temperature dependence is quite small and so we give metal-insulator phase diagrams for $T=0$. The dependence of the hole density at the transition on the impurity layer separation d for GaAs is shown in Fig. 4. The impurity density is fixed at $n_i=0.5\times 10^{11}$ cm^{-2}. We compare our results with the observation of the transition in Ref. 2 in a GaAs sample. Our curve is consistent with this measurement. The phase boundary is sensitive to d because of the exponential factor in $U_{\text{imp}}(q)$. This suppresses carrier-impurity scattering for short wavelengths $q \gg d$. For the residual long wavelength scattering the correlations are always weak. Thus, when d is large the correlations play a relatively less important role in the localization.

The phase diagram in Fig. 5 plots the critical electron density in Si at the transition as a function of impurity density n_i. The impurity layer separations are $d=0$ and $5a_0^\star$. We also show experimental data points for the position of the transition in Si.[13] Again, our predicted phase boundary agrees with these observations. On our curve the electron-impurity scattering becomes weaker as the critical electron-density decreases. Thus at the transition point the electron mobility will increase as the electron density decreases. This is consistent with observations.[1,13]

We conclude that correlations and impurity scattering do mutually affect the localization transition. Finite temperatures tend to suppress correlations and this slightly reduces the critical carrier density for localization to occur by an amount that becomes significant for temperatures of the order of the Fermi temperature.

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